

Myrcene

123-35-3 | DTXSID6025692

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.20

Global applicability domain: Inside

Local applicability domain index: 6.07e-01

Confidence level: 7.12e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Myrcene

Measured: 4.17

Predicted: 4.20

[Image not found](#)

sec-Butylbenzene

Measured: 4.57

Predicted: 4.31

[Image not found](#)

o-Diethylbenzene

Measured: 3.72

Predicted: 4.29

[Image not found](#)

1,3-Diethylbenzene

Measured: 4.57

Predicted: 4.29